

# Author index

- Abad-Zapatero, C. 865  
 Abagyan, R. 249  
 Adams, G.P. 301  
 Adams, J.A. 609  
 Adib-Conquay, M. 859  
 Adman, E.T. 153  
 Adzhubei, A.A. 615  
 Aert, R. 159  
 Akutsu, N. 39  
 Albrechtsen, B. 1063  
 Alexander, R.S. 975  
 Alfthan, K. 725  
 Amadei, A. 1129  
 Amati, V. 403  
 Ammendola, S. 31  
 Anderson, F. 1189  
 Anderson, H.W. 1063  
 Appelt, K. 677  
 Åqvist, J. 1137  
 Aramaki, H. 1259  
 Argos, P. 21, 1011  
 Atkinson, H.J. 1303  
 Avrameas, S. 859  
  
 Baase, W.A. 1017  
 Baker, K.C. 59  
 Baker, P.J. 147  
 Bakker, A.H.F. 293, 1295  
 Baláz, S. 809  
 Banerjee, S. 1189  
 Barnett, J. 275  
 Bayley, H. 491  
 Beato, M. 71  
 Benhabiles, N. 829  
 Benner, S.A. 457  
 Bennett, G.L. 1057  
 Bennett, S. 91  
 Beppu, T. 153  
 Berendsen, H.J.C. 1129  
 Betts, A.H. 593  
 Beveridge, A.J. 135  
 Bi, R.-C. 211  
 Björkstén, J. 5  
 Blättler, W.A. 481  
 Boberg, J. 501, 505  
 Bohr, H. 389  
 Bookman, M.A. 301  
 Boutonnet, N.S. 647  
 Brady, J.W. 1145  
 Brasseur, R. 829  
 Brem, R. 1205  
 Brennan, C. 865  
 Brenner, S.E. 319  
 Briggs, G.S. 59  
 Brinkmann, U. 1323  
 Britton, K.L. 147  
 Brown, A.M. 397  
 Brukner, I. 283  
  
 Cambria, A. 551  
 Carter, D.C. 471  
 Carter, P. 1057  
 Cattaneo, A. 403  
 Chan, C.M.W. 193  
 Chan, H.S. 1205  
 Chao, Y. 211  
 Chen, H.-m. 575  
 Chen, L. 865, 1049  
 Chen, M.-J. 1233  
 Chiaraluce, R. 1287  
 Chiu, C.Y. 463  
 Chou, K.-C. 425  
  
 Christianson, D.W. 975  
 Christodoulou, C. 859  
 Chu, N.-M. 211  
 Clark, B.F.C. 1267  
 Collins, J. 45  
 Collura, V.P. 1197  
 Colotti, G. 593  
 Connerton, I.F. 59  
 Consalvi, V. 1287  
 Coutinho, P. 1049  
 Craik, C.S. 275  
 Cummings, N.J. 59  
 Cygler, M. 835  
  
 Daggett, V. 1117  
 Danson, M.J. 583  
 Davies, P.L. 843  
 De Benedetti, P.G. 557  
 De Maeyer, M. 815  
 de Vlieg, J. 21  
 de Vos, W.M. 117, 1287  
 Dealwis, C.G. 865  
 Declerck, N. 1029  
 Degtyarenko, K.N. 737  
 Delagrave, S. 237  
 delCardayré, S.B. 261  
 DeLisi, C. 1081  
 Demetrius, L. 791  
 Desideri, A. 551  
 Desmet, J. 815  
 Dhople, V.M. 315  
 Dill, K.A. 769, 1205  
 Doi, H. 1171  
 Dunkel, R. 71  
  
 Eggen, R.I.L. 1287  
 Egmond, M.R. 21  
 Eisenberg, D. 627  
 Elce, J.S. 843  
 Eldridge, M.D. 1197  
 Elliott, G. 471  
 Ely, K.R. 823  
 Emahazion, T. 1163  
 Engberg, J. 1063  
 Engel, P.C. 147  
 Eroshkin, A.M. 167  
  
 Fand, I. 301  
 Fanelli, F. 557  
 Farber, G.K. 1189  
 Farkas, Ö. 925  
 Fastrez, J. 451  
 Fernández, J.A. 1253  
 Fierke, C.A. 975  
 Findlay, J.B.C. 1129  
 Finkelstein, A.V. 207, 883  
 Firth, M.A. 1197  
 Fischer, D. 981  
 Flanagan, K. 109  
 Ford, C. 575, 1049  
 Fox, T. 53  
 Francis, D.M. 193  
 Freedman, R.B. 59  
 Freer, S.T. 677  
 Fu, Z.-Q. 1233  
 Fujita, I. 935  
 Fuxreiter, M. 925  
  
 Gaillardin, C. 1029  
 Gallet, X. 829  
 Galvano, M. 551  
 Galzitskaya, O.V. 883  
  
 Garnier, J. 1029  
 Gauthier, S. 843  
 Geerling, A.C.M. 1287  
 Gershoni, J.M. 143, 717  
 Gerstein, M. 319, 329  
 Gilbert, M. 859  
 Gileva, I.P. 167  
 Gish, G. 609  
 Gö, N. 353  
 Godzik, A. 409  
 Goffin, V. 1215  
 Goldmacher, V.S. 481  
 Goldman, E.R. 237  
 Goldstein, R.A. 641  
 Goodenough, P.W. 59  
 Goodfellow, J.M. 109  
 Goormaghtigh, E. 249  
 Goraj, K. 249  
 Gould, H.J. 193  
 Griffin, J.H. 1253  
 Guild, B.C. 481  
  
 Hansen, L.K. 379  
 Hansson, T. 1137  
 Hara, T. 711  
 Hardman, K.D. 749  
 Harrison, R.W. 1233  
 Hartley, R.W. 497  
 Hashimoto, Y. 1023  
 Hayashi, Y. 763  
 Hecht, H.-J. 45  
 Hegadorn, C. 843  
 Heimstad, E.S. 379  
 Hemminki, A. 185  
 Henklein, P. 471  
 Henneke, C.M. 13  
 Henry, A.J. 193  
 Heringa, J. 21  
 Herzberg, O. 1275  
 Hide, M. 193  
 Ho, J.X. 471  
 Hoffrén, A.-M. 185, 443  
 Höhne, W. 471  
 Holewa, B. 733  
 Horinouchi, S. 153  
 Houbrechts, A. 249  
 Hough, D.W. 583  
 Houston, L.L. 301  
 Howard, A.J. 749  
 Hubbard, S.J. 1011  
 Hudziak, R.M. 301  
 Hunter, M.J. 1177  
 Huston, J.S. 301  
 Hwang, J.-K. 363  
  
 Imamura, M. 1171  
 Imberty, A. 699  
 Imoto, T. 201, 1023  
 Incani, O. 31  
 Ippolito, J.A. 975  
 Ishino, Y. 1171  
 Islam, S.A. 513  
  
 Janacek, S. 809  
 Jespers, L. 451  
 Jin, D. 301  
 Johansen, L.K. 1063  
 Johnson, M.S. 873  
 Joseph-McCarthy, D. 1103  
 Joyet, P. 1029  
 Jung, S.-H. 1323  
  
 Kadono, S. 763  
 Kamyinina, T.P. 167  
 Kanppik, A. 81  
 Karginova, E.A. 167  
 Karplus, M. 1103  
 Karshikoff, A. 243  
 Kattinger, D. 471  
 Kato, H. 711  
 Kato, I. 1171  
 Kaufman, S.E. 463  
 Kawaguchi, J. 763  
 Keeling, K. 471  
 Keller, D.A. 893  
 Kiefer, L.L. 975  
 Kirschner, K. 535  
 Klein-Hitpaß, L. 733  
 Klimenko, L.V. 63  
 Knudsen, C.R. 1267  
 Kodandapani, R. 823  
 Koga, H. 201  
 Kolinski, A. 225  
 Komeiji, Y. 935  
 Komives, E.A. 1177  
 Koshi, J.M. 641  
 Kramer, A. 471  
 Krek, C.E. 481  
 Kretsinger, R.H. 63  
 Kuipers, O.P. 117  
 Kukimoto, M. 153  
 Kumagai, I. 1153  
 Kunicki, T.J. 823  
 Kurochkina, N. 437  
 Kuroda, Y. 97  
 Kuwajima, K. 1153  
  
 Ladino, C.A. 481  
 Laminet, A.A. 301  
 Lamproye, A. 249  
 Laramée, L. 835  
 Laskowski, R.A. 127  
 Lasters, I. 815  
 Loughton, C.A. 615  
 Lebbink, J.H.G. 1287  
 Lebedev, L.R. 167  
 Lee, B. 437, 1323  
 Lee, D.-H. 91  
 Leung, R. 275  
 Lewin, M. 829  
 Li, A. 1117  
 Li, J. 1197  
 Liao, W.-F. 363  
 Lim, C. 565  
 Linacre, J. 527  
 Liu, S. 301  
 Lomakin, A.S. 167  
 Lorenz, P. 733  
 Luo, J. 513  
  
 Mackay, G.A. 193  
 Maeda, Y. 201  
 Maggiora, G.M. 425  
 Mainfroid, V. 249  
 Mäkinen, M.-L. 185  
 Manchester, J.I. 801  
 Mandeck, W. 865  
 Mannervik, B. 1163  
 Marcus, E. 893  
 Marino, M. 551  
 Marotti, K.R. 293  
 Martial, J.A. 249, 1215  
 Martin, A.C.R. 389, 1093  
 Martin, S. 147

# Author index

- Mason, P. 53  
Matsushima, N. 63  
Matthews, B.W. 1017  
May, A.C.W. 873  
McCammon, J.A. 397, 663, 915  
McCartney, J.E. 301  
McDonald, I.K. 217  
McDonald, S.M. 915  
McGlone, M.L. 609  
McPherson, M.J. 1303  
Medvedkin, V.N. 63  
Meininger, D.P. 1177  
Mele, A. 31  
Menziani, M.C. 557  
Milik, M. 225  
Min, H.Y. 463  
Mitin, Y.V. 63  
Miyazawa, S. 999  
Mizuguchi, K. 353  
Mordenti, J. 1057  
Moreau, B. 249  
Moriyama, H. 763  
Mort, J.S. 53  
Mucovic, M. 497  
Muir, J.M. 583  
Mullenbach, G.T. 463  
Muro, M. 39  
Murphy, J.R. 1317  
Murray, C.W. 1197
- Nagaraj, R. 315  
Nair, S.K. 975  
Nakayama, S. 63  
Nakhei, H. 733  
Náray-Szabó, G. 925  
Negro, A. 175  
Neidle, S. 615  
Niermann, T. 535  
Nieuwenbroek, N.M.E. 1295  
Nikolov, Z. 1049  
Nilsson, B. 601  
Nilsson, J. 601  
Nishioka, T. 711, 1075  
Nishiyama, M. 153  
Nord, K. 601  
Nosoh, Y. 39  
Nugel, E. 471  
Numata, K. 39, 763  
Nussinov, R. 981  
Nygren, P.-Å. 601
- O'Connor, J. 1243  
Ochagavia, M.-E. 647  
Oda, J. 711, 1075  
Ohnuki, T. 153  
Okoniewska, M. 835  
Ollis, D.L. 135  
Onodera, K. 763  
Ophir, R. 143  
Oppermann, H. 301  
Ornstein, R.L. 801, 893  
Osaka, G. 1057  
Oshima, T. 39, 763  
Owens, R.J. 193
- Panayotou, G. 527  
Pardani, A. 593  
Pastan, I. 1323  
Pastor, N. 543  
Pawson, T. 609
- Pederson, K. 91  
Pereboev, A.V. 167  
Ignat'ev, G.M. 167  
Pérez, S. 699  
Perez-Prat, E.M. 1153  
Permyakov, E.A. 63  
Petsko, G.A. 905, 1103  
Pettersson, K. 185  
Philippopoulos, M. 565  
Planas, A. 939  
Plückthun, A. 81  
Policelli, F. 551  
Pomès, R. 663  
Poncin, A. 249  
Pons, J. 939  
Porstmann, T. 471  
Poteete, A.R. 593  
Pratt, K.A. 13, 59  
Préaux, G. 249  
Pregel, M.J. 1309  
Price, S.L. 109
- Querol, E. 939  
Quirk, D.J. 261
- Raines, R.T. 261  
Rajalakshmi, N. 1039  
Raucci, G. 31  
Recktenwald, A. 835  
Reczko, M. 389  
Reed, C. 1233  
Rehberg, E.F. 293  
Reilly, P.J. 575  
Rein, R. 893  
Reiter, Y. 1323  
Revell, D.F. 59  
Ribó, M. 261  
Rice, D.W. 147  
Richelle, J. 647  
Ridgway, J.B.B. 1057  
Robben, J. 159  
Rollema, H.S. 117  
Rooman, M.J. 647, 849  
Rosenberg, S. 463  
Royer, Jr., W.E. 593  
Rüker, F. 471  
Russell, R.J.M. 583  
Rutter, W.J. 261  
Ruysschaert, J.-M. 249  
Ryffel, G.U. 733
- Sakurai, M. 763  
Salakoski, T. 501, 505  
Sampson, E. 1317  
Saqi, M. 1069  
Scandurra, R. 1287  
Schneider-Mergener, J. 471  
Schomburg, D. 45  
Schrage, J.D. 835  
Selbig, J. 339  
Shen, S.-H. 1309  
Shi, J. 193  
Shibata, M. 893  
Shoichet, B.K. 1017  
Siezen, R.J. 117  
Sigal, E. 275  
Simon, I. 417  
Sizmann, D. 725  
Skaper, S.D. 175  
Skolnick, J. 225
- Sloane, D.L. 275  
Smalás, A.O. 379  
Smith, D.D.S. 13  
Smith, T.J. 1275  
Soares, C.M. 5  
Söderlund, H. 185, 725  
Solar, I. 717  
Soman, K.V. 397  
Soumillion, P. 451  
Stafford, III, W.F. 301  
Sternber, M.J.E. 513  
Stigler, R.-D. 471  
Stirk, H.J. 1093  
Storer, A.C. 53, 1309  
Stratton-Thomas, J.R. 463  
Suck, D. 283  
Suhai, S. 389  
Summerford, C.M. 593  
Summers, N.L. 1215  
Sumner, I.G. 13  
Sun, S. 1205  
Sundaram, P.V. 1039  
Suns, S. 769  
Suske, G. 71  
Sutherland, J. 1317  
Sutton, B.J. 193  
Suyama, M. 1075  
Suzuki, M. 1, 319, 329, 1259  
Szardenings, M. 45  
Szilágyi, A. 779
- Tai, M.-S. 301  
Takahashi-Fujii, A. 1171  
Takkinen, K. 185, 725  
Tanaka, N. 763  
Tanaka, T. 711  
Tapia, O. 5  
Taylor, J.S. 1145  
Taylor, M.A.J. 59  
Teeri, T.T. 185, 443, 725  
Teleman, O. 185, 443, 1253  
Teo, B. 1145  
Thomas, D.Y. 835  
Thomas, P.D. 769  
Thomas-Soumamon, A. 829  
Thornton, J.M. 127, 217, 1093  
Toda, K. 1093  
Tomizawa, H. 1023  
Tramontano, A. 31, 403  
Trosset, J.-Y. 1029  
Tsai, C.-J. 981  
Turley, S. 153  
Tusnády, G. 417  
Tusnády, G.E. 417
- Uchiyama, H. 1153  
Ueda, T. 201  
Uemori, T. 1171  
Uhlén, M. 601  
Urwin, P.E. 1303
- Vajda, S. 1081  
Vakser, I.A. 371  
van Aalten, D.M.F. 1129  
Van der Schueren, 159  
vanderSpek, J.C. 1317  
Vasel, B. 45  
Vehniäinen, M. 185  
Verhasselt, P. 159  
Verheijen, J.H. 293, 1295
- Verkhivker, G. 677  
Vernet, T. 835  
Vervoort, J. 451  
Vihinen, M. 501, 505  
Villafranca, J.E. 677  
Villoutreix, B.O. 1253  
Vince, J.W. 843  
Volckaert, G. 159  
von Heijne, G. 693  
von Strandmann, E.P. 733  
von Strandmann, R.P. 733  
Voss, E.W. 749  
Vriend, G. 71
- Walker, B. 491  
Wallace, A. 31  
Wallace, A.C. 127  
Wallin, E. 693  
Walshaw, J. 109  
Wang, X.-g. 147  
Warren, G.L. 905  
Warwick, J. 1243  
Watanabe, K. 1153  
Waterfield, M.D. 527  
Weber, I.T. 1233  
Weiner, L.M. 301  
Weinhold, E.G. 457  
Weinstein, H. 543  
Weng, Z. 1081  
Werge, T.M. 403  
Westhead, D.R. 1197  
White, C.E. 1177  
White, L.R. 1177  
Whitlow, M. 749  
Widersten, M. 1163  
Willson, R.C. 663, 915  
Wilmanns, M. 627  
Wilson, D.B. 1145  
Wilson, K.P. 1017  
Wodak, S.J. 647, 849  
Wolf, E. 283  
Wolfson, H. 981  
Wong, W.L.T. 1057  
Wood, J.F. 749  
Wu, J. 1233
- Xiang, Y. 565  
Xue, Y.-N. 1233
- Yagi, N. 319, 329, 1259  
Yamada, H. 201, 1023  
Yamagishi, A. 39, 763  
Yamato, I. 935  
Yilmaz, S. 1163  
Yokel, E.M. 261  
Young, R.J. 193  
Youvan, D.C. 237
- Zapata, G. 1057  
Závodszy, P. 779  
Zawadzke, L.E. 1275  
Zhang, C.-T. 425  
Zhang, X.-j. 1017  
Zhu, Z.-Y. 103  
Ziomek, E. 835  
Zoidl, C. 733  
Zvelebil, M.J.J.M. 527

# Subject index

- Accessible surface area**  
used to estimate hydrophobic effect 437
- Acetylcholine receptor**  
cassette mutagenesis of acetylcholine binding site 143
- Active site**  
of *Clostridium symbiosum* glutamate dehydrogenase, site-directed mutagenesis 147
- $\alpha_1\beta$ -Adrenergic receptor**  
molecular dynamics simulation of signal transduction in 557
- Alcaligenes faecalis***  
pseudoazurin interaction with nitrite reductase, effect of site-directed mutagenesis 153
- Alcohol dehydrogenase**  
*Sulfolobus solfataricus*, thermostability, effect of mutation 31  
yeast, site-directed mutagenesis 457
- Alginate synthesis**  
*Pseudomonas*, regulation of 63
- Algorithm**  
for identifying domains of proteins 513
- Algorithms**  
for dealing with gaps in protein sequence comparison 1075
- Alkaline phosphatase**  
*E. coli* D153G mutant of 865
- Amino acid analogues**  
incorporation of 7-azatryptophan into lysozyme 451
- Amino acids**  
determining hydrophobicity parameters 1081  
relationships based on protein building features 417
- Aminoacyl tRNA binding**  
site-directed mutagenesis of elongation factor Tu 1267
- $\alpha$ -Amylase**  
*Bacillus licheniformis*, altering thermostability of 1029
- Anti-receptor antibody**  
crystal structure of OPG2 fragment 823
- Antibodies**  
artificial, strategy for constructing 601  
bacterial secretion of mouse IgM Fab fragment 859  
engineering disulphide-linked single-chain Fv dimers 301  
engineering linear F(ab')<sub>2</sub> fragments 1057  
improving labelling properties of anti-hAFP antibody Fab fragment 185  
prediction of hypervariable CDR-H3 loop using neural network 389  
recombinant, mutations affecting folding 81  
stabilizing Fv fragments by engineering disulphide bonding 1323
- Antibody-antigen binding**  
free energy simulations of HyHEL-10/HEL complex 663  
interaction of anti-HIV-1 gp41 Fab fragment with its peptide epitope 471  
pK<sub>a</sub> of HyHEL-5-hen egg lysozyme complex 915
- Antimicrobial peptides**  
based on *Staphylococcus aureus*  $\delta$ -toxin 315
- L-Arabinose isomerase**  
*E. coli* 1189
- Arachidonic acid**  
positional specificity of lipoxygenase binding 275
- Arc**  
binding to DNA 1
- Archaea**  
*Pyrococcus furiosus* citrate synthase 583
- Asparagine**  
application of hydrogen bonding analysis in X-ray crystallography to orientate side chains 217
- Aspartyl bonds**  
in *Aspergillus awamori* glucoamylase, site-directed mutagenesis of 575
- Aspergillus***  
deletion analysis of glucoamylase starch-binding domain 1049
- 7-Azatryptophan**  
incorporation into lysozyme 451
- Bacillus caldotenax***  
DNA polymerase, amino acid sequence required for 5'→3' exonuclease activity 1171
- Bacillus licheniformis***  
 $\alpha$ -amylase, altering thermostability of 1029  
1,3-1,4- $\beta$ -glucanase, role of disulphide bond in stability of 939
- Bacillus stearothermophilus***  
lactate dehydrogenase, molecular dynamics simulation of protein loop closure 565
- Bacillus subtilis***  
isopropylmalate dehydrogenase, thermostability of chimera with *Thermus thermophilus* enzyme 39  
subtilisin E, crystal structure of complex with phenylmethanesulphonyl fluoride 211
- Barnase**  
*in vivo* detection of low-activity mutants 497
- $\alpha/\beta$ -Barrel**  
structural stability, effect of  $\beta$ -residue packing 249
- ( $\alpha/\beta$ )<sub>8</sub>-Barrel enzymes**  
evolutionary relationships of 809
- c-ErbB-2**  
(sFv')<sub>2</sub> version of monoclonal antibody against 301
- C4b-binding protein**  
interaction with protein S 1253
- Calpain II**  
recombinant, improving expression of 843
- Cam**  
and Tet, DNA binding domains of 1259
- CAP**  
DNA bending by 329
- Carbonic anhydrase II**  
structure of His94→Asp mutant 975
- Cassette mutagenesis**  
efficient design of combinatorial library 143  
of *E. coli* trp repressor 935
- Catalytic triad**  
Cys-His-Asp, in diene lactone hydrolase 135  
of *Geotrichum candidum* lipase 835
- Cathepsin B**  
alteration of subsite specificity by mutation 53
- Cavities**  
within globular proteins, detection of 1011
- Cellulases**  
*Thermomonospora fusca* endocellulase E2, modelling substrate binding 1145
- Cellulose-binding domain**  
fungal, molecular dynamics simulation of 443
- Cephalosporins**  
third generation, hydrolysis by engineered *Staphylococcus aureus*  $\beta$ -lactamase 1275
- Chloramphenicol acetyltransferase**  
reactivation of misfolding mutant as strategy for positive selection 159
- Chymotrypsin inhibitor 2**  
solution structure 1117
- Ciliary neurotrophic factor**  
fusion protein with diphtheria toxin, characterization of 175
- Citrate synthase**  
from the hyperthermophile *Pyrococcus furiosus* 583
- Classification**  
of proteins by complete linkage clustering [letter] 501
- Clostridium difficile***  
glutamate dehydrogenase 1287
- Clostridium symbiosum***  
site-directed mutagenesis of glutamate dehydrogenase active site 147
- CLUSPROT**  
for analysis of determinants of subtilisin thermostability 21
- Co-operativity**  
of proteins, model for investigating 593
- Combinatorial cassette mutagenesis**  
of *Rhodobacter capsulatus* LH2 light-harvesting protein 237
- Combinatorial library**  
efficient design of 143  
solid-phase gene assembly strategy for constructing 601
- Complete linkage clustering**  
used to identify protein families [letter] 501
- Complex formation**  
docking algorithm for low-resolution structures 371

## Subject index

### Conformational search

- minimum perturbation, for modelling mutant structure of triose phosphate isomerase 1103

### Contact matrix

- use for protein structure prediction 339

### Covalent modification

- alters thermostability of papain 1039
- of  $\alpha$ -haemolysin, restores pore-forming activity 491

### Cystatin C

- inhibition of cysteine proteases, residues affecting 53

### Cystatins

- role of N-terminal region of oryzacystatin I 1303

### Cysteine proteases

- alteration of subsite specificity by mutation 53
- recombinant pro-regions of papain and papaya proteinase IV inhibit mature enzymes 59

### Cysteine proteinase inhibitors

- role of N-terminal region of oryzacystatin I 1303

### Cystic fibrosis transmembrane conductance regulator

- prediction of epitopes using molecular modelling 829

### Cytochrome P450cam

- molecular dynamics simulation of pentachloroethane dehalogenation by 801

### Dead-end elimination

- for determining global minimum energy conformation 815
- using fuzzy end elimination algorithm 893

### Dehalogenation

- of pentachloroethane by cytochrome P450cam 801

### Dialysis

- for effective renaturation of urea-denatured lysozyme 201

### Dienelactone hydrolase

- substrate-induced activation of 135

### Digoxin

- (sFv')<sub>2</sub> version of monoclonal antibody against 301

### Diphtheria toxin

- fusion protein with ciliary neurotrophic factor, characterization of 175
- fusion with simian interleukin 15 1317

### Distantly related proteins

- protein sequence comparison of 1075

### Disulphide bonding

- for stabilizing Fv fragments 1323
- role in stability of 1,3-1,4- $\beta$ -glucanase 939

### DNA bending

- by CAP 329

### DNA binding domains

- of Cam and Tet 1259

### DNA binding proteins

- DNA recognition by helix-turn-helix proteins 329
- interaction of transcription factors with DNA [review] 319
- $\beta$ -sheet, binding to DNA 1

### DNA binding specificity

- electrostatic analysis of TATA box binding protein mutants 543

### DNA polymerase

- Bacillus caldopenax*, amino acid sequence required for 5'→3' exonuclease activity 1171

### DNase I

- interaction with DNA, altering sequence selectivity 283

### Docking

- algorithm for low-resolution structures 371

### Domain-domain interaction

- in tissue-type plasminogen activator hybrids with urokinase-type plasminogen activator 1295

### Domains

- algorithm for identifying 513

### Double dynamic programming

- compared with iterative algorithm 1197

### Elastase inhibitors

- comparison of predictive strategies for protein design 45

### Electrostatic analysis

- of TATA box binding protein mutants 543

### Electrostatic interactions

- algorithm for calculation of multiple site titration curves 243

### Electrostatic potential field

- of Cu,Zn superoxide dismutase 551

### Electrostatics

- determining pK<sub>a</sub> of HyHEL-5-hen egg lysozyme complex 915
- model for interaction of water with phenylalanine 109
- molecular modelling of xylose isomerase catalysis 925
- role in C4b-binding protein interaction with protein S 1253

### Elongation factor Tu

- site-directed mutagenesis 1267

### Endocellulase E2

- Thermomonospora fusca*, modelling substrate binding 1145

### Endoplasmic reticulum

- determinants of zein retention in 91

### Enzymes

- classification by thermodynamic parameters 791

### Epitopes

- of cystic fibrosis transmembrane conductance regulator, prediction of using molecular modelling 829

### Escherichia coli

- cassette mutagenesis of *trp* repressor 935
- magnesium binding by mutant alkaline phosphatase 865

### Evolution

- of sugar isomerases 1189

### Evolutionary relationships

- of ( $\alpha/\beta$ )<sub>8</sub>-barrel enzymes 809

### 5'→3' Exonuclease

- activity of *Bacillus caldopenax* DNA polymerase, amino acid sequence required for 1171

### Expression vector

- for phage display 1063

### F(ab')<sub>2</sub> fragments

- linear, engineering 1057

### Fab fragment

- expression vector for phage display 1063
- of anti-hAFP antibody, improving labelling properties 185
- of mouse IgM, bacterial secretion of 859

### $\alpha$ -Fetoprotein

- improving labelling properties of anti-hAFP antibody Fab fragment 185

### Fibronectin

- crystal structure of cell-binding type III module 823

### Fluorescein

- crystal structure of anti-fluorescein Fab 749

### Four-helix bundle protein

- as candidate vaccine against HIV 167

### v-Fps

- kinase domain of 609

### Free energy calculations

- of ligand-protein complexes 677

### Free energy simulations

- of HyHEL-10/HEL antibody-antigen binding 663

### Fusion protein

- diphtheria toxin-CNTF, characterization of 175

### Fuzzy classification

- for prediction of secondary structure 505

### Fuzzy clustering

- for predicting structural classes of proteins 425

### Fuzzy end elimination

- algorithm for finding global energy minimum 893

### Fv dimers

- disulphide-linked single-chain, engineering 301

### Fv fragments

- stabilizing by engineering disulphide bonding 1323

### G-protein coupled receptors

- model of binding site in substance P receptor and anti-SP antibody 403
- N-terminal tails of 693

### Gaps

- in protein sequence comparison, algorithms for dealing with 1075

### Gene inversion

- as basis for *in vivo* detection of low-activity barnase mutants 497

### Genetic algorithm

- for predicting tertiary structure 769
- for protein structure comparison 873

### Geotrichum candidum

- lipase, redesigning active site of 835

- Global minimum energy conformation**  
 attaining, effect of temperature 883  
 determining using dead-end elimination 815  
 finding using fuzzy end elimination algorithm 893
- Globular proteins**  
 detection of cavities within 1011  
 predicting structural classes using fuzzy clustering 425
- 1,3-1,4- $\beta$ -Glucanase**  
*Bacillus licheniformis*, role of disulphide bond in stability of 939
- Glucoamylase**  
*Aspergillus*, deletion analysis of starch-binding domain 1049  
*Aspergillus awamori*, site-directed mutagenesis of thermolabile aspartyl bonds in 575
- Glutamate dehydrogenase**  
*Clostridium symbiosum*, site-directed mutagenesis of active site 147  
*Pyrococcus furiosus* and *Clostridium difficile*, effects of domain swapping 1287
- Glutamine amidotransferase**  
 predicting secondary structure 535
- Glutathione synthetase**  
*E.coli*, site-directed mutagenesis of 711
- Glutathione transferase A1-1**  
 creating nickel binding site by site-directed mutagenesis 1163
- D-Glyceraldehyde-3-phosphate dehydrogenase**  
*Thermotoga maritima*, structural basis for thermostability 779
- Glycosylation**  
 effect of elimination of glycosylation sites on human IgE Fc region binding to IgE receptors 193  
 of ribonuclease A expressed in *S.cerevisiae* 261  
 stereochemistry of *N*-glycosylation sites 699
- Greek key jellyroll**  
*de novo* design of  $\beta$ -sheet 13
- Growth hormone**  
 interaction with receptor 1215
- GTPase mechanism**  
 of elongation factor Tu 1267
- Haemoglobin**  
 dimeric, bacterial expression of 593
- $\alpha$ -Haemolysin**  
 pore-forming activity restored by covalent modification 491
- Haemolytic activity**  
 of *Staphylococcus aureus*  $\delta$ -toxin, determinants of 315
- Helical proteins**  
 with stable folds, design of 97
- $\alpha$ -Helix**  
 composition of in thermophiles 905
- Helix-turn-helix proteins**  
 DNA recognition by 329
- HisA**  
 inverse protein folding by residue pair preference profile method 627
- Histidine**  
 application of hydrogen bonding analysis in X-ray crystallography to orientate side chains 217
- Histidine tag**  
 to aid purification of recombinant calpain II 843
- Histidine-tagged proteins**  
 monoclonal antibody for detecting [Protocol] 733
- Histone-like proteins**  
 binding of (AAKP)<sub>n</sub> and (KKSP)<sub>n</sub> to DNA 63
- HIV**  
 four-helix bundle protein as candidate vaccine 167
- HIV-1**  
 binding free energy of proteinase inhibitor 1137  
 interaction of anti-HIV-1 gp41 Fab fragment with its peptide epitope 471  
 predicting binding affinity of protease 677
- HMG box protein**  
 homology modelling of Sox-5 615
- Homology modelling**  
 determining global minimum energy conformation using dead-end elimination 815  
 for analysis of thermostability 779  
 of Sox-5 HMG box protein 615  
 of tumour necrosis factor  $\alpha$  receptor binding 1233  
 of vicilin solubility 1243
- Homology studies**  
 amino acid relationships based on protein building features 417
- Hydrogen bonding**  
 application of hydrogen bonding analysis in X-ray crystallography to orientate side chains 217
- Hydrophobic core**  
 designing sequences to fold with 1205  
 of  $\alpha$ -lactalbumin, effect of mutation 1153
- Hydrophobic effect**  
 estimating 437  
 model for interaction of water with phenylalanine 109
- Hydrophobicity parameters**  
 of amino acids, determining 1081
- Immunoassay**  
 improving labelling properties of anti-hAFP antibody Fab fragment 185
- Immunoglobulin E**  
 effect of elimination of glycosylation sites on human IgE Fc region binding to IgE receptors 193
- Immunotoxin**  
 recombinant ricin, expression and secretion from myeloma 481
- Interleukin 15**  
 simian, fusion with diphtheria toxin 1317
- Inverse protein folding**  
 by residue pair preference profile method 627  
 designing sequences to fold with hydrophobic cores 1205
- Inverse protein folding problem, 409**
- 3-Isopropylmalate dehydrogenase**  
 altering thermostability using site-directed mutagenesis 763
- Isopropylmalate dehydrogenase**  
 thermostability of *Thermus thermophilus* chimera with *Bacillus subtilis* enzyme 39
- Iterative algorithm**  
 compared with double dynamic programming 1197
- Kringle 2 domain**  
 effect of position in tissue-type plasminogen activator 293
- $\alpha$ -Lactalbumin**  
 effect of mutation in hydrophobic core 1153
- $\beta$ -Lactamase**  
*Staphylococcus aureus*, engineered to hydrolyse third generation cephalosporins 1275
- Lactate dehydrogenase**  
*Bacillus stearothermophilus*, molecular dynamics simulation of protein loop closure 565
- Lactococcus lactis**  
 homology modelling of nisin-NisP interaction 117
- Leader peptidases**  
 homology modelling of nisin-NisP interaction 117
- Ligand-protein interaction**  
 predicting binding affinity of HIV-1 protease 677
- Ligand-receptor interaction**  
 docking algorithm for low-resolution structures 371
- Light-harvesting protein**  
*Rhodobacter capsulatus* LH2, combinatorial cassette mutagenesis 237
- LIGPLOT**  
 for 2-D representation of protein-ligand interaction 127
- Linker modification**  
 effect of linker modification on molecular stability of single chain antibody 717
- Lipase**  
*Geotrichum candidum*, redesigning active site of 835  
 human pancreatic, catalytic triad of 835
- Lipoxygenase**  
 positional specificity, effect of site-directed mutagenesis 275
- Long loops**  
 role in protein folding 1093
- Low complexity sequences**  
 structural analysis of 1069
- Lysozyme**  
 free energy simulations of HyHEL-10/HEL antibody-antigen binding 663  
 hen egg-white, enhancing thermostability 1023  
 incorporation of 7-azatryptophan 451



## Subject index

- pK<sub>a</sub> of HyHEL-5-hen egg lysozyme complex** 915  
T4, enhancing thermostability of 1017  
urea-denatured, effective renaturation of 201
- M3-muscarinic receptor**  
molecular dynamics simulation of signal transduction in 557
- Magnesium binding**  
by *E. coli* D153G mutant alkaline phosphatase 865
- Membrane proteins**  
N-terminal tails of G-protein coupled receptors 693
- MetJ**  
binding to DNA 1
- Mnt**  
binding to DNA 1
- Molecular dynamics simulation**  
for investigating solution structure of chymotrypsin inhibitor 2 1117  
of cellular retinol binding protein 1129  
of enzyme-catalysed pentachloroethane dehalogenation 801  
of fungal cellulose-binding domain 443  
of HIV-1 proteinase inhibitor 1137  
of pore closing in porin 5  
of protein loop closure 565  
of signal transduction in  $\alpha_{1B}$ -adrenergic receptor and m3-muscarinic receptor 557  
used to study mobility of bovine and salmon trypsin 379
- Molecular modelling**  
for prediction of cystic fibrosis transmembrane conductance regulator epitopes 829
- Molten globule state**  
of  $\alpha$ -lactalbumin, stability of 1153
- Monoclonal antibody**  
for detecting histidine-tagged proteins [Protocol] 733
- Monte Carlo optimization**  
for protein side-chain prediction 363
- Monte Carlo simulation**  
of protein folding 883
- Multiple linkage clustering**  
for protein structure comparison 647
- Myeloma**  
expression and secretion of recombinant ricin immunotoxin 481
- Neural network**  
for protein side-chain contact mapping 225  
for protein side-chain prediction 363  
used for prediction of hypervariable CDR-H3 loop 389
- Nickel binding site**  
in glutathione transferase A1-1, creating by site-directed mutagenesis 1163
- Nisin**  
homology modelling of nisin-NisP interaction 117
- Nitrite reductase**  
interaction with pseudoazurin, effect of site-directed mutagenesis 153
- Oryzacystatin I**  
role of N-terminal region in cysteine proteinase inhibition 1303
- P450-containing monooxygenase systems**  
structural domains of [Review] 737
- Packing defects, 1011**
- Papain**  
and papaya proteinase IV, recombinant pro-regions inhibit mature enzymes 59  
covalent modification alters thermostability 1039
- Papaya proteinase IV**  
and papain, recombinant pro-regions inhibit mature enzymes 59  
residues affecting inhibition of by cystatin C 53
- Pentachloroethane**  
dehalogenation by cytochrome P450cam 801
- Peptide-DNA binding**  
binding of (AAKP)<sub>n</sub> and (KKSP)<sub>n</sub> to DNA 63
- Peptide epitope library**  
used to study interaction of anti-HIV-1 gp41 Fab fragment with its peptide epitope 471
- Phage display**  
expression vector for 1063
- Phagemid display**  
of urokinase plasminogen activator EGF-like domain 463
- Phenylalanine**  
model for interaction with water 109
- Phenylmethanesulphonyl fluoride**  
crystal structure of complex with subtilisin E 211
- Phosphopeptides**  
analysis of interaction with SH2 domain 527
- Pichia pastoris**  
expression system for human thrombomodulin 1177
- pK**  
calculation of: algorithm for calculation of multiple site titration curves 243
- Pore**  
 $\alpha$ -haemolysin pore-forming activity restored by covalent modification 491  
predicting secondary structure of potassium channel H5 pore 397
- Pore closing**  
in porin, mechanism of 5
- Porin**  
mechanism of pore closing 5
- Positional specificity**  
of lipoxygenase, effect of site-directed mutagenesis 275
- Positive selection**  
using reactivation of chloramphenicol acetyltransferase misfolding mutant 159
- Potassium channel**  
predicting secondary structure of H5 pore 397
- Pro-regions**  
of papain and papaya proteinase IV, inhibit mature enzymes 59
- Probability alignment, 999**
- Progesterone**  
model for binding to uteroglobin 71
- Prolactin**  
human, interaction with receptor 1215
- Protease**  
HIV-1, predicting binding affinity of 677
- Protease inhibitors**  
comparison of predictive strategies for protein design 45
- Protein-DNA interaction**  
interaction of transcription factors with DNA [review] 319
- Protein-ligand interaction**  
2-D representation using LIGPLOT 127
- Protein-protein interaction**  
pseudoazurin interaction with nitrite reductase, effect of site-directed mutagenesis 153
- Protein Data Bank**  
structural classes within 981
- Protein design**  
*de novo* design of Greek key jellyroll motif 13  
of elastase inhibitors 45  
of four-helix bundle protein as candidate vaccine against HIV 167  
of helical proteins with stable folds 97
- Protein families**  
classification by complete linkage clustering [letter] 501
- Protein folding**  
database-derived potentials for [Review] 849  
estimating hydrophobic effect 437  
inverse protein folding problem 409  
Monte Carlo simulation of 883  
mutations affecting folding of recombinant antibodies 81  
role of long loops 1093
- Protein loop closure**  
molecular dynamics simulation of *Bacillus stearothermophilus* lactate dehydrogenase loop 565
- Protein S**  
interaction with C4b-binding protein 1253
- Protein sequence comparison**  
of distantly related proteins 1075
- Protein side-chain contact mapping**  
using neural network 225
- Protein side-chain prediction**  
using neural network and simulated annealing 363
- Protein structure**  
comparing using spatial arrangement of secondary structure elements 353
- Protein structure classification**  
algorithms for 981

- Protein structure comparison**  
by multiple linkage clustering 647  
genetic algorithm for 873
- Protein structure prediction**  
by threading method 1197  
database-derived potentials for protein folding [Review] 849  
genetic algorithm for predicting tertiary structure 769  
of hypervariable CDR-H3 loop, using neural network 389  
predicting secondary structure of glutamine amidotransferase 535  
predicting secondary structure of potassium channel H5 pore 397  
predicting structural classes using fuzzy clustering 425  
prediction of secondary structure using fuzzy classification 505  
using contact matrix 339
- Protein targeting**  
determinants of zein retention in endoplasmic reticulum 91
- Protein tyrosine phosphatase 1C**  
regulation of 1309
- Proteinase inhibitor**  
HIV-1, binding free energy of 1137
- Pseudoazurin**  
interaction with nitrite reductase, effect of site-directed mutagenesis 153
- Pseudomonas**  
regulation of alginate synthesis 63
- Pyrococcus furiosus**  
citrate synthase 583  
glutamate dehydrogenase 1287
- Reaction rate**  
of enzymes, relationship with substrate specificity 791
- Receptor binding**  
by prolactin and growth hormone 1215  
by tumour necrosis factor  $\alpha$  1233
- Renaturation**  
effective renaturation of urea-denatured lysozyme 201
- Residue pair preference profile**  
for inverse protein folding 627
- Retinol binding protein**  
cellular, molecular dynamics simulation of 1129
- RGD molecules**  
common molecular scaffold for 823
- Rhodobacter capsulatus**  
combinatorial cassette mutagenesis of LH2 light-harvesting protein 237
- Ribonuclease**  
*in vivo* detection of low-activity barnase mutants 497
- Ribonuclease A**  
cDNA cloning and mutagenesis 261
- Ricin**  
expression and secretion of recombinant immunotoxin from myeloma 481
- Scapharca**  
bacterial expression of dimeric haemoglobin 593
- Secondary structure**  
evaluating methods for prediction of 103  
of glutamine amidotransferase, predicting 535  
prediction of using fuzzy classification 505
- Secondary structure elements**  
spatial arrangement of, used to compare protein structure 353
- Secretion**  
bacterial, of mouse IgM Fab fragment 859  
of whole human IgE Fc region 193
- Seed storage proteins**  
vicilin 1243
- Sequence alignment**  
999
- Sequence homology**  
method for deriving substitution matrix 641
- Sequence selectivity**  
of DNase I interaction with DNA, altering 283
- Serine proteases**  
Cys-His-Asp catalytic triad in diene lactone hydrolase 135  
homology modelling of nisin-NisP interaction 117
- SH2 domain**  
analysis of interaction with phosphopeptides 527
- $\beta$ -Sheet**  
*de novo* design of Greek key jellyroll motif 13  
experimental test of predicted stability parameters [letter] 207  
interaction with DNA 1
- Signal transduction**  
in  $\alpha_1\beta$ -adrenergic receptor and m3-muscarinic receptor, molecular dynamics simulation of 557
- Simulated annealing**  
Monte Carlo optimization, for protein side-chain prediction 363
- Single chain antibody**  
effect of linker alteration 725  
effect of linker modification on molecular stability 717
- Site-directed mutagenesis**  
effect on pseudoazurin interaction with nitrite reductase 153  
of anti-hAFP antibody Fab fragment 185  
of *Clostridium symbiosum* glutamate dehydrogenase active site 147  
of *E. coli* glutathione synthetase 711  
of elongation factor Tu 1267  
of hen egg-white lysozyme 1023  
of lipoxygenase, effect on positional specificity 275  
of *Staphylococcus aureus*  $\beta$ -lactamase 1275  
of thermolabile aspartyl bonds in *Aspergillus awamori* glucoamylase 575  
of yeast alcohol dehydrogenase 457  
to alter sequence selectivity of DNase I 283  
to alter thermostability of  $\alpha$ -amylase 1029  
to create nickel binding site in glutathione transferase A1-1 1163  
using to alter thermostability of 3-isopropylmalate dehydrogenase 763
- Solid-phase gene assembly**  
strategy for constructing combinatorial library 601
- Solute partitioning**  
for determining hydrophobicity parameters of amino acids 1081
- Sox-5**  
homology modelling of 615
- src homology 2 domains**  
role regulation of protein tyrosine phosphatase 1C 1309
- Stability**  
experimental test of predicted  $\beta$ -sheet stability parameters [letter] 207
- Staphylococcus aureus**  
 $\beta$ -lactamase, engineered to hydrolyse third generation cephalosporins 1275  
 $\delta$ -toxin, determinants of haemolytic activity 315
- Starch-binding domain**  
of *Aspergillus* glucoamylase, deletion analysis 1049
- Structural domains**  
of P450-containing monooxygenase systems [Review] 737
- Substance P**  
model of binding site in receptor and anti-SP antibody 403
- Substitution matrix**  
method for deriving 641
- Substrate binding**  
*Thermomonospora fusca* endocellulase E2, modelling 1145
- Substrate recognition**  
*Clostridium symbiosum* glutamate dehydrogenase, effect of site-directed mutagenesis of active site 147
- Substrate specificity**  
of enzymes, relationship with reaction rate 791  
of yeast alcohol dehydrogenase, altering using site-directed mutagenesis 457
- Subtilisin E**  
crystal structure of complex with phenylmethanesulphonyl fluoride 211
- Subtilisin**  
determinants of thermostability 21
- Sugar isomerases**  
evolution of 1189
- Sulfolobus solfataricus**  
alcohol dehydrogenase thermostability, effect of mutation 31
- Superoxide dismutase**  
modelling 3-D structure of Cu,Zn SOD 551
- Symmetry**  
4-fold and 8-fold, role in structural stability of  $\alpha/\beta$ -barrel 249
- TIM barrel proteins**  
glutamine amidotransferase predicted to have TIM barrel fold 535
- T4**  
lysozyme, enhancing thermostability of 1017
- Tandem repeats**  
binding of (AAKP) $_n$  and (KKSP) $_n$  to DNA 63
- TATA box binding protein**  
electrostatic analysis of mutants 543
- Tet**  
and Cam, DNA binding domains of 1259

## Subject index

### Thermodynamic parameters

classification of enzymes by 791

### Thermolability

of aspartyl bonds in *Aspergillus awamori* glucoamylase 575

### *Thermomonospora fusca*

endocellulase E2, modelling substrate binding 1145

### Thermophiles

$\alpha$ -helix composition in 905

### Thermostability

citrate synthase from the hyperthermophile *Pyrococcus furiosus* 583

determinants of in subtilisin 21

of hen egg-white lysozyme, enhancing 1023

of 3-isopropylmalate dehydrogenase, altering using site-directed mutagenesis 763

of papain, altering by covalent modification 1039

of *Pyrococcus furiosus* and *Clostridium difficile* glutamate dehydrogenase 1287

of *Sulfolobus solfataricus* alcohol dehydrogenase, effect of mutation 31

of T4 lysozyme, enhancing 1017

of *Thermotoga maritima* D-glyceraldehyde-3-phosphate dehydrogenase, structural basis 779

of *Thermus thermophilus* isopropylmalate dehydrogenase chimera with *Bacillus subtilis* enzyme 39

### *Thermotoga maritima*

D-glyceraldehyde-3-phosphate dehydrogenase, structural basis for thermostability 779

### *Thermus thermophilus*

isopropylmalate dehydrogenase, thermostability of chimera with *Bacillus subtilis* enzyme 39

### Threading

method of protein structure prediction 1197

### Threading algorithm

for addressing inverse protein folding problem 409

### Three-helix bundle protein

surface mutagenesis of 601

### Thrombomodulin

human, expression in *Pichia pastoris* 1177

### Tissue-type plasminogen activator

effect of position of Kringle 2 domain 293

hybrids with urokinase-type plasminogen activator 1295

### $\delta$ -Toxin

*Staphylococcus aureus*, determinants of haemolytic activity 315

### Transcription factors

DNA binding domains of Cam and Tet 1259

interaction with DNA [review] 319

possible binding sites for TFIIA and TFIIB 543

### TraY

binding to DNA 1

### *Trichoderma reesei*

cellulose-binding domain, molecular dynamics simulation of 443

### Triose phosphate isomerase

modelling mutant structure 1103

### *trp* repressor

*E.coli*, cassette mutagenesis of 935

### Trypsin

bovine and salmon, mobility of, studied using molecular dynamics simulation 379

### Tumour necrosis factor $\alpha$

receptor binding 1233

### Tyrosine protein kinase

kinase domain of v-fps 609

### Urea

effective renaturation of urea-denatured lysozyme 201

### Urokinase plasminogen activator

yeast expression and phagemid display of EGF-like domain 463

### Urokinase-type plasminogen activator

hybrids with tissue-type plasminogen activator 1295

### Uteroglobin

model for binding of progesterone 71

### Vicilin

homology modelling of solubility 1243

### X-ray crystallography

application of hydrogen bonding analysis to orientate side chains 217

of subtilisin E-PMSF complex 211

### Xylose isomerase

molecular modelling of catalysis 925

### Zein

determinants of retention in endoplasmic reticulum 91

### Zinc binding site

in carbonic anhydrase II 975

of *Sulfolobus solfataricus* alcohol dehydrogenase, effect of mutation on thermostability 31



